Anisole, 2,3,4,5,6-pentachloro-

Other names:	Benzene, pentachloromethoxy-
	Methyl pentachlorophenate
	Methyl pentachlorophenyl ether
	Pentachloroanisole
	Pentachloromethoxybenzene
	2,3,4,5,6-Pentachloroanisole
	Methyl pentachlorophenyl ester
	NCI-C56520
	Pentachlorophenyl methyl ether
	PCP, Methyl ether
	Phenol, pentachloro-, methylated
Inchi:	InChI=1S/C7H3Cl5O/c1-13-7-5(11)3(9)2(8)4(10)6(7)12/h1H3
InchiKey:	BBABSCYTNHOKOG-UHFFFAOYSA-N
Formula:	C7H3Cl5O
SMILES:	COc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	280.36
CAS:	1825-21-4

Physical Properties

Property code	Value	Unit	Source
gf	-92.33	kJ/mol	Joback Method
hf	-219.55	kJ/mol	Joback Method
hfus	28.16	kJ/mol	Joback Method
hvap	61.10	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.962		Crippen Method
mcvol	152.800	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	1672.00		NIST Webbook
rinpol	291.70		NIST Webbook
rinpol	1754.20		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1721.00		NIST Webbook
rinpol	1741.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1724.00		NIST Webbook

rinpol	1741.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	291.70		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	1754.20		NIST Webbook
ripol	2315.00		NIST Webbook
ripol	2257.00		NIST Webbook
ripol	2298.00		NIST Webbook
ripol	2245.00		NIST Webbook
ripol	2279.00		NIST Webbook
ripol	2313.00		NIST Webbook
ripol	2245.00		NIST Webbook
ripol	2315.00		NIST Webbook
tb	620.71	K	Joback Method
tc	863.72	K	Joback Method
tf	429.50	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.72	J/mol×K	620.71	Joback Method
cpg	290.46	J/mol×K	823.22	Joback Method
cpg	285.54	J/mol×K	782.71	Joback Method
cpg	280.19	J/mol×K	742.21	Joback Method
cpg	274.43	J/mol×K	701.71	Joback Method
cpg	268.27	J/mol×K	661.21	Joback Method
cpg	294.95	J/mol×K	863.72	Joback Method
dvisc	0.0002057	Pa×s	620.71	Joback Method
dvisc	0.0002391	Pa×s	588.84	Joback Method
dvisc	0.0002827	Pa×s	556.97	Joback Method
dvisc	0.0003412	Pa×s	525.11	Joback Method
dvisc	0.0004219	Pa×s	493.24	Joback Method
dvisc	0.0005372	Pa×s	461.37	Joback Method
dvisc	0.0007089	Pa×s	429.50	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1825214&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume